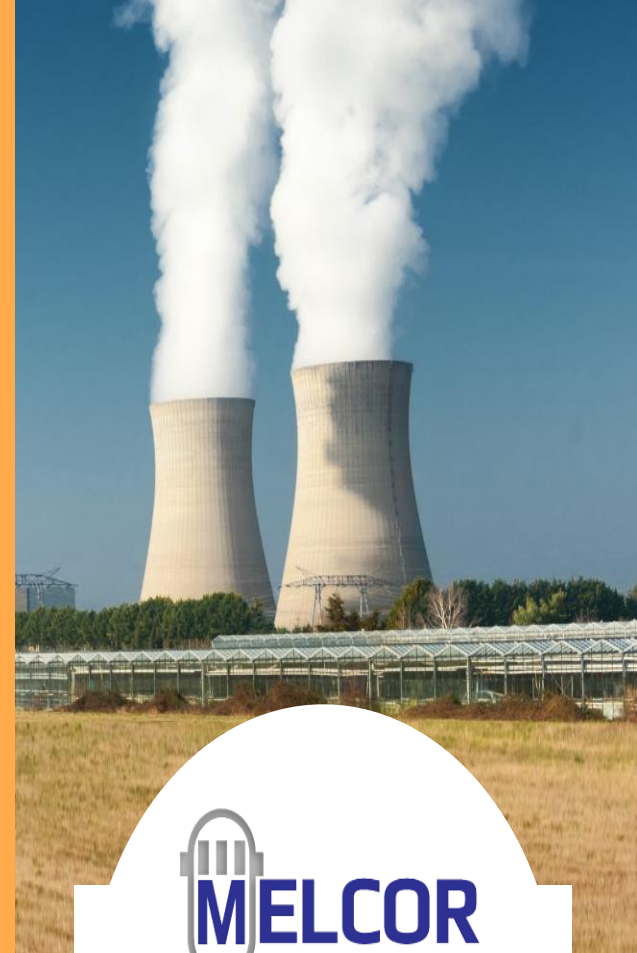


*Securing the future of Nuclear Energy*



# MELCOR Materials

2024 European MELCOR Users' Group Meeting

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SAND2024-03742PE



# Overview



## Discuss MELCOR “materials” in a broad sense

- Hydrodynamic materials (light water, non light water, noncondensable gases)
  - Specific heat, enthalpy, and density from equation of state
  - Thermal conductivity, viscosity, & binary diffusion coefficient - Material Properties (MP) package
- Non-hydrodynamic materials (accessed via MP package)
  - Specific heat, enthalpy, and density as functions of temperature
  - Melting temperature, heat of fusion, and (constant) average density
  - Solid but sometimes subject to melting, oxidation, and eutectic interactions

## Code defaults – “Built-in” materials

- 37 MP materials – usually in core and heat structures, can be augmented from default
- All non light water hydrodynamic materials (light water, NCG package library gases)

## User defined – New materials

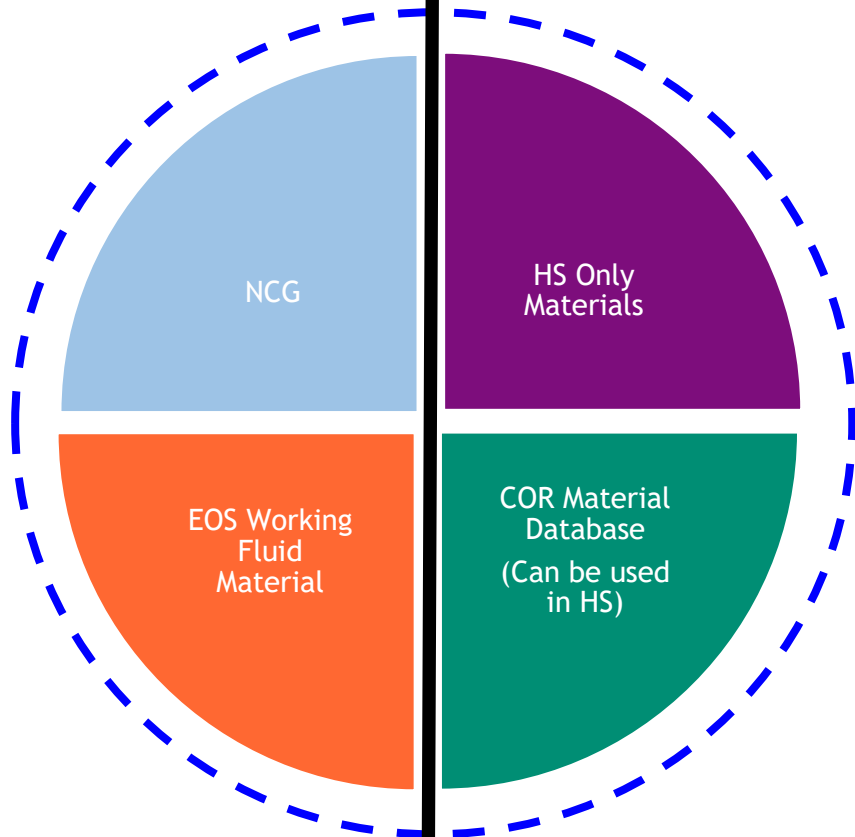
- MP for use as (usually) heat structure or core component materials
    - User Defined Materials (UDM) in MP
    - Select specialized models in other physics packages (e.g. eutectics and generic oxidation)
  - EOS/CVH/CVT for hydrodynamic (condensable) materials
  - NCG package for user-declared noncondensable gases as hydrodynamic materials
-

# Diagram of MELCOR Materials



## MELCOR Materials Database

Fluids ← → Solids



Fluids ← → Solids

- AR
- H2
- HE
- AR
- D2
- O2
- CO2
- CO
- N2
- NO
- N2O
- NH3
- C2H2
- CH4
- C2H4
- WATER**
- STEAM**
- NON-LWR**

- Zircaloy (ZR)
- Zirconium Oxide (ZRO2)
- Zirconium Oxide (ZRO2-INT)
- Uranium Dioxide (UO2)
- Uranium Dioxide (UO2-INT)
- Stainless Steel (SS)
- Stainless Steel Oxide (SSOX)
- Boron Carbide (B4C)
- Boron Carbide (B4C-INT)
- Silver-Indium-Cadmium (AGINC)
- Uranium Metal (UMETL)
- Graphite (GRAPH)
- Concrete (CON)**
- Aluminum (ALUM)
- Aluminum Oxide (AL2O3)
- Cadmium (CADM)
- Stainless Steel 304 (SS304)
- Lithium Aluminum (LIAL)
- Uranium Aluminum (UAL)
- Carbon Steel (CS)

# Material Defaults - Models & Built-In Data



## Hydrodynamic materials

- Viscosity
  - Tables in MP database (water, steam, air, H<sub>2</sub>, D<sub>2</sub>)
  - M2.1 default (and M2.2) to use equation fit for He, air, N<sub>2</sub>, O<sub>2</sub>, Ar
  - Optional viscosity data from Chapman-Enskog model
    - Model uses Leonard-Jones potential parameters from constants in MP package database
    - Steam, air, H<sub>2</sub>, He, Ar, D<sub>2</sub>, O<sub>2</sub>, CO<sub>2</sub>, CO, N<sub>2</sub>, NO, N<sub>2</sub>O, Ammonia, Acetylene, Methane, Ethylene
- Thermal Conductivity
  - Tabular data from MP database ( Water, steam, air)
  - M2.1 default (and M2.2) to use equation fit for He, air, N<sub>2</sub>, O<sub>2</sub>, Ar
  - Thermal conductivity from viscosity (Eucken) if no table or fit
- Binary Diffusion Coefficients - Chapman-Enskog model
- Standard models used for mixtures

## Non-hydrodynamic Materials in MP database

- Specific heat, enthalpy, and density as  $f(T)$  from tables; default tables
  - Melting temperature, heat of fusion, and (constant) average density from constants
-

# Material Defaults - MELGEN Input



Built-in material data can be modified by user input

- Non-hydrodynamic (MP Package)
  - Can replace constants in MP database
  - Can replace default tables with user tables from TF package
  - Can use a control function for thermal conductivity
- Hydrodynamic and noncondensable (NCG Package - thermal conductivity & viscosity)
  - Default is to use equation fits to tables described in RM, where available
  - Can replace with user defined tables from Tabular Functions package
  - Can use control functions
  - Can specify Chapman-Enskog model for viscosity (and Eucken eqn for thermal conductivity)

New material properties can be defined (MP, EOS/CVH/CVT Packages)

- Non-hydrodynamic materials (MP) for use in HS or COR packages
  - Hydrodynamic and noncondensable - NCG allows user-defined
    - For these, must also define thermal conductivity, viscosity, and Leonard-Jones coefficients for binary diffusion coefficient
  - Hydrodynamic and condensable - EOS package (and CVH/CVT)
    - Change the condensable working fluid of the calculation - non-LWR or fusion applications
    - Configure multiple condensable working fluids in a calculation (EOS networks)
    - ThermoProperty Fluid (TPF) files and viscosity/conductivity data
-

# MELGEN Material Plots



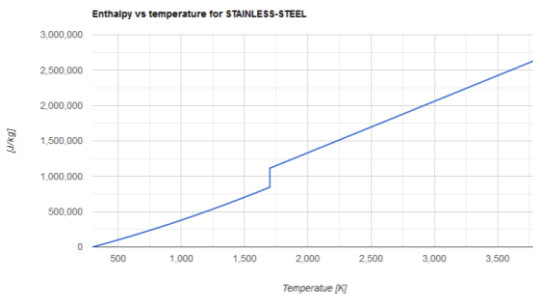
## MATERIAL PROPERTIES PACKAGE

Show Properties for fiberglass

Show Properties for STAINLESS-STEEL

Show Properties for ZIRCALOY

- Materials
  - User-defined materials
  - Default Materials
- Properties
  - Thermal conductivity
  - Enthalpy
  - Heat capacity

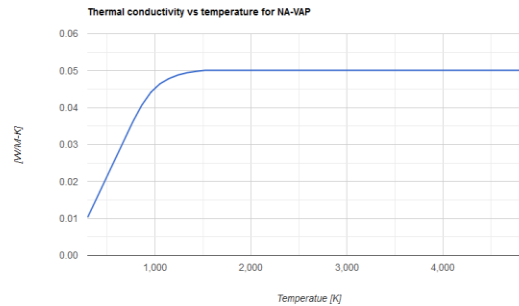


## NON CONDENSIBLE GAS PACKAGE

Show Properties for POOL

Show Properties for NA-VAP

- Viscosity
- Thermal conductivity
- Internal energy

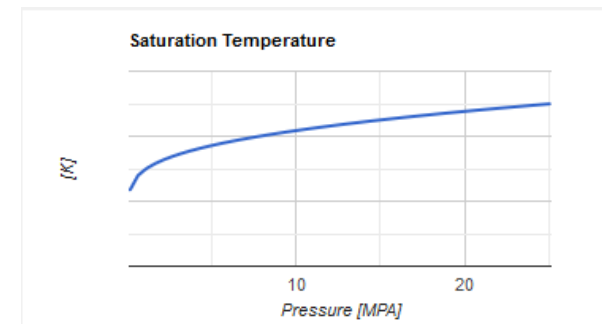


No Input Required by User

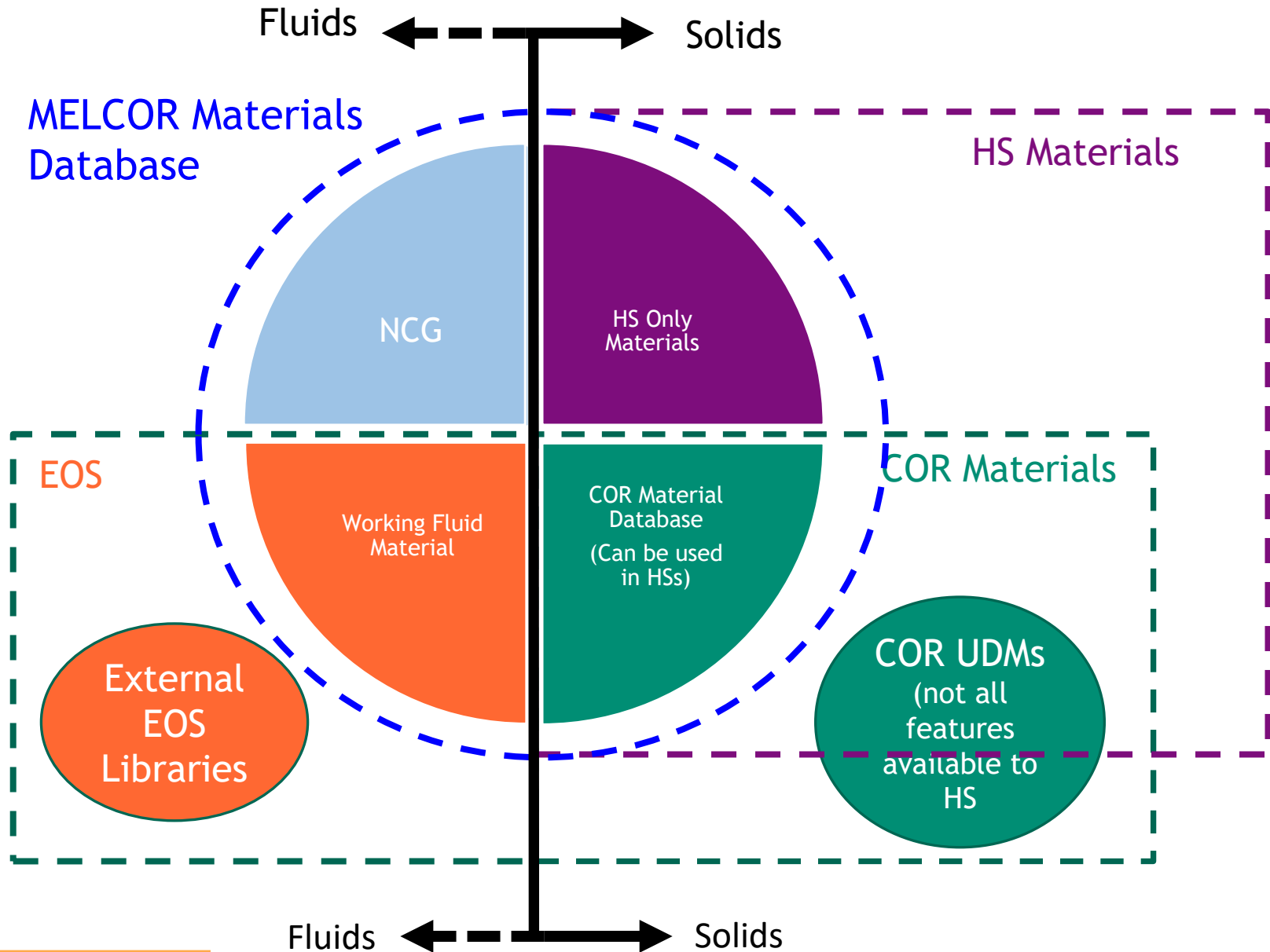
## Equation of State PACKAGE

EOS Properties for Na

- Saturation Pressure
- Saturation Temperature
- Liquid Density at saturation
- Vapor density at saturation
- Liquid specific enthalpy at saturation pressure
- Vapor specific enthalpy at saturation pressure
- Liquid specific heat
- Vapor specific heat



# Diagram of MELCOR Materials - NCG



# NCG – Enthalpy and Internal Energy



## Enthalpy:

$$h(T) = \int_{T_n}^T \left( c_v(T') + \frac{R}{w} \right) dT' + h_{form}$$

## Internal Energy:

$$e(T) = \int_{T_n}^T c_v(T') dT' + e_{form}$$

## Fit to $C_v$ :

$$c_v(T) = c_{v0} + c_{v1}T + c_{v2}T^2 + c_{v3}T^3 + \frac{c_{vsqrt}}{\sqrt{T}} + \frac{c_{vm1}}{T} + \frac{c_{vm2}}{T^2}$$

## Implementation:

$$e(T) = e_0 + c_{v0}T + \frac{1}{2}c_{v1}T^2 + \frac{1}{3}c_{v2}T^3 + \frac{1}{4}c_{v3}T^4 + 2c_{vsqrt}\sqrt{T} + c_{vm1}\ln(T) - \frac{c_{vm2}}{T}$$

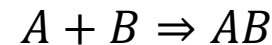
## Energy of formation:

$$e_0 = e_{form} - c_{v0}T_n - \frac{1}{2}c_{v1}T_n^2 - \frac{1}{3}c_{v2}T_n^3 - \frac{1}{4}c_{v3}T_n^4 - 2c_{vsqrt}\sqrt{T_n} - c_{vm1}\ln(T_n) + \frac{c_{vm2}}{T_n}$$

$T_{low} \leq T \leq T_{up}$   $e(T)$  extrapolated outside that range using the constant limiting specific heat at  $T_{low}$  or  $T_{up}$

- All heats of formation of compounds are included in the enthalpy functions, as in JANAF tables. The advantage is that all heats of reaction are implicitly contained in the enthalpy functions.
- Therefore, chemical reactions (such as gas combustion simulated by the Burn package) can be treated simply as changes in the masses of various materials; the associated heat effects are accounted for automatically through the equations of state.

## Chemical Reaction:



## Heat of reaction:

$$Q_R(T) = h_A(P, T) + h_B(P, T) - h_{AB}(P, T)$$



# NCG – Chapman-Enskog Equation & Solution to Boltzmann Equation



## Pure Gas

$$\mu_i = 2.6693 \times 10^{-6} \frac{\sqrt{1000 M T}}{\sigma^2 \Omega_v} \quad \text{kg/m-s}$$

$M$  = molecular weight (kg/mol)

$T$  = gas temperature (K)

$\sigma$  = collision diameter ( $\text{\AA} \equiv 10^{-10}\text{m}$ )

$\Omega_v$  = collision integral

$$= 2.785 \left( \frac{T^*}{0.3} \right)^{-0.4} \quad T^* < 0.3 \text{ (extrapolated)}$$

$$= f(T^*) \text{ from Table 5.1 below} \quad 0.3 \leq T^* < 100$$

$$= 0.5882 \left( \frac{T^*}{100} \right)^{-0.145} \quad T^* \geq 100$$

$$T^* = \frac{k T}{\varepsilon}$$

$\varepsilon/k$  = characteristic energy/Boltzmann's constant (K)

## Gas Mixture

$$\mu_{mix} = \sum_{i=1}^n \frac{y_i \mu_i}{\sum_{j=1}^n y_j \phi_{ij}}$$

$y_i$  = mole fraction of gas  $i$

$\mu_i$  = viscosity of pure gas  $i$  (see Section 5.2)

$$\phi_{ij} = \frac{[1 + (\mu_i / \mu_j)^{1/2} (M_j / M_i)^{1/4}]^2}{[8(1 + M_i / M_j)]^{1/2}}$$

$$= \frac{1}{\sqrt{8}} \left( \frac{M_j}{M_i} \right) \left( \frac{M_i}{M_j + M_i} \right)^{1/2} \left[ \left( \frac{M_i}{M_j} \right)^{1/4} + \left( \frac{\mu_i}{\mu_j} \right)^{1/2} \right]^2$$

$M_i$  = molecular weight of gas  $i$  (kg/mol), set by the NCG package

- Only two parameters (Lennard-Jones) are required,  $\sigma$  and  $\varepsilon$
- When Chapman-Enskog is invoked, it is also used in calculating thermal conductivity utilizing the Eucken Correction

$$\lambda_i = \left( C_{vi} + \frac{9R}{4M_i} \right) \mu_i \quad (W/m-K)$$

# NCG – Properties on NCG\_PRP Table



```
NCG ID N2 !Default Properties Used
NCG_ID O2 !Redefined Properties
NCG_PRP 3 ! N MPNAME MPVALUE
          1 CV0 3000.0
          2 TLOW 200.0
```

Redefine Properties for O2 which exists in database

```
NCG_ID MyGas !User-defined NCG
```

Error message if \_PRP card is missing

**ERROR: RECORD NCG\_PRP for user defined NCG:  
MYNCG IS REQUIRED**

```
NCG ID MyGas !User-defined NCG
NCG_PRP 2
          1 VIS C-E
          2 THC C-E
```

Error message if \_PRP input is incomplete

**Error in table: NCG\_PRP NCG: MYNCG  
All 14 properties for user NCG should be present**

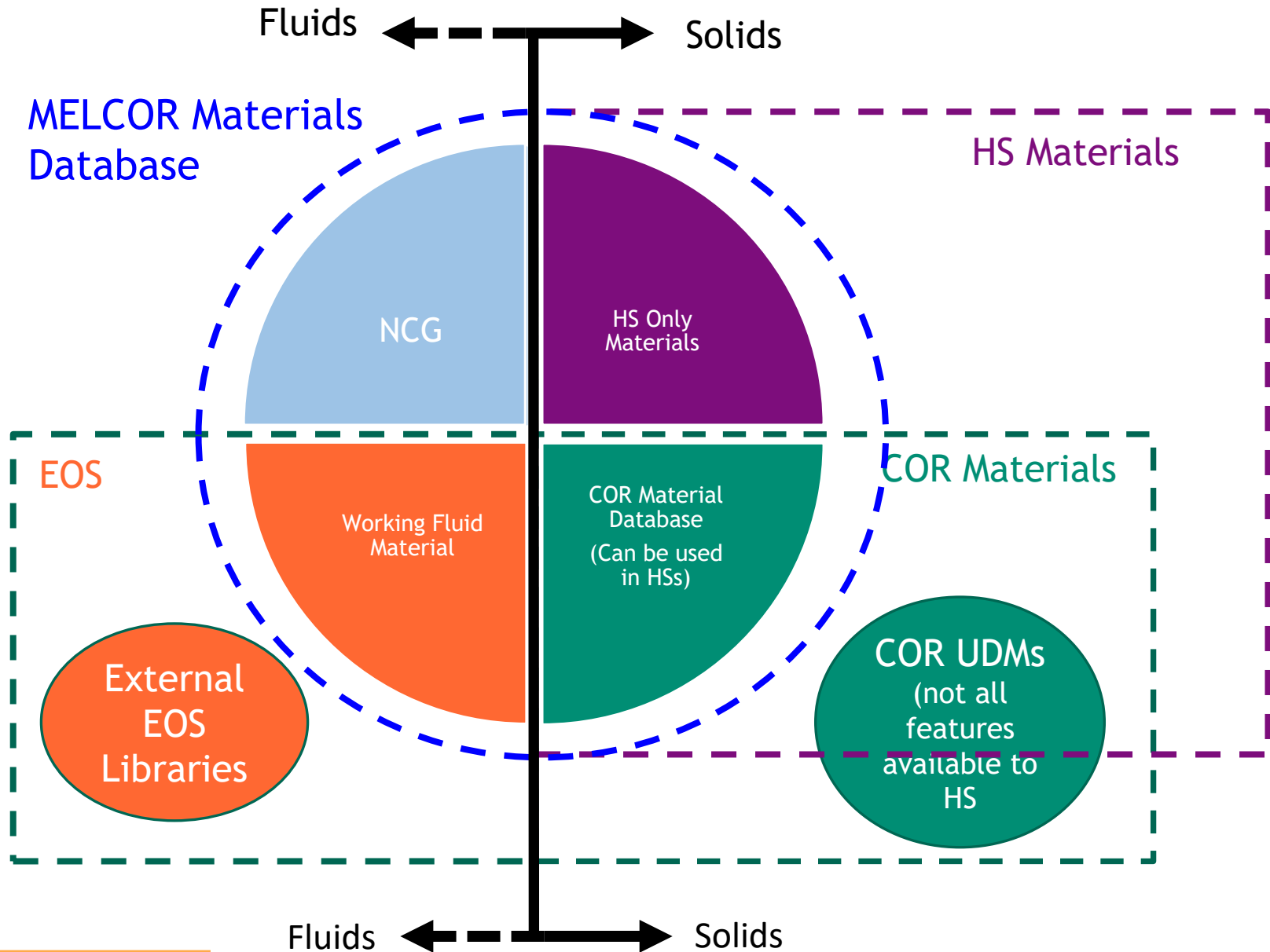
```
NCG ID MyGas !User-defined NCG
NCG_PRP 16
          1 SIG 2.827
          2 EPS 59.7
          3 CV0 -17849.0
          4 CV1 11.28298
          5 CV2 -2.1081958e-3
          6 CV3 1.5635602E-7
          7 CVSQRT 865616.
          8 CVM1 -8188058.3
          9 CVM2 1.925734E8
          10 TLOW 100.
          11 TUP 6000.
          12 WM 0.0020162
          13 EF 0.
          14 SZ 0.
          15 VIS C-E
          16 THC C-E
```

Material Property Name	Units	Physical Interpretation
CV0	J/(kg K)	$c_{v0}$ coefficient in $c_v(T)$
CV1	J/(kg K <sup>2</sup> )	$c_{v1}$ coefficient in $c_v(T)$
CV2	J/(kg K <sup>3</sup> )	$c_{v2}$ coefficient in $c_v(T)$
CV3	J/(kg K <sup>4</sup> )	$c_{v3}$ coefficient in $c_v(T)$
CVSQRT	J/(kg $\sqrt{K}$ )	$c_{vsqrt}$ coefficient in $c_v(T)$
CVM1	J/kg	$c_{vm1}$ coefficient in $c_v(T)$
CVM2	(J K)/kg	$c_{vm2}$ coefficient in $c_v(T)$
TLOW	K	$T_{low}$ lowest temperature for fit to $c_v(T)$
TUP	K	$T_{up}$ highest temperature for fit to $c_v(T)$
WM	kg/mol	molecular weight
EF	J/kg	$e_f$ energy of formation
SZ	J/(kg K)	$s_0$ entropy at natural temperature (not used currently)
SIG	Å(10 <sup>-10</sup> m)	Lennard-Jones potential parameter,
EPS	K	Lennard-Jones potential parameter, $\epsilon/k$

User-defined NCG



# Diagram of MELCOR Materials - EOS



# EOS Package



EOS is now a MELCOR package with its own Users' Guide and input records

- Concerns hydrodynamic, condensable materials occupying either/or pool/atmosphere
- Incorporates and is backwards-compatible with former methods of invoking a working fluid and an EOS in a calculation (e.g. EXEC READFLUID)
- No required input for built-in water or single condensable via TPF and READFLUID
- Required input when multiple condensable hydrodynamic materials exist
- Interfaces closely with CVH and CVT and acts like a property library

EOS functions pervade the code:

- Touch points with COR, CVH, FL, and HS permit multiple condensables
- Packages specialized to water applications will generate an error if non-water condensable is associated with them (e.g., BUR, CAV, CND, FCL, FDI, PAR, SPR)
- Special treatments here and there, e.g. RN hygroscopic model and sensitivity coefficient sets

One default built-in (improved implementation for water), TPFs otherwise

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# EOS – Property Libraries



Sodium properties/EOS based on SIMMER-III

MELEOS (user defined library) under development

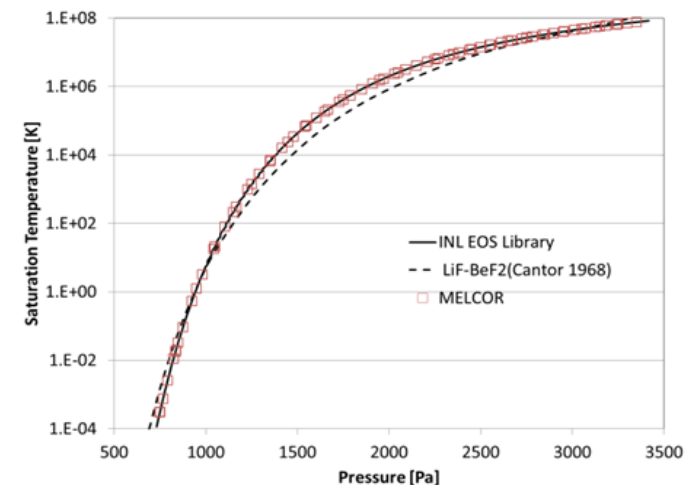
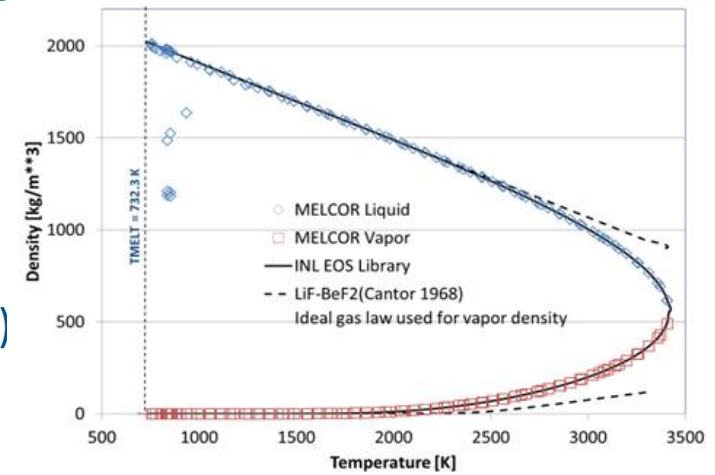
Multi-EOS facilitated by EOS package

EOS implements properties/EOS from INL FSD

- Parametric Helmholtz Free Energy with 8 terms
- INL/CON-16-38063 on Pb-Li (Humrickhouse, Merrill)

Materials:

Fluid Name	Database Type	Database Name	Default File Name
Water	Built-in	Water	—
Water	TPF	H2O	tpfh2o
Hydrogen		H2	tpfh2
Lithium		Li	tpfli
Potassium		K	tpfk
Helium		He	tpfhe
Nitrogen		N2	tpfn2
Sodium		Na	tpfna
Sodium-Potassium		NaK	tpfnak
Lithium-Lead		LiPb	tpflipb
Fluoride-Lithium-Beryllium		FLiBe	tpffi



# EOS – MELGEN Input



## Define hydrodynamic condensable fluids and “EOS networks”

### EOS\_FLUID\_ID – User Fluid Name and Sequence Number

Required

This record defines a unique, user-defined name for the fluid and a user-defined sequence number.

- (1) EOS fluid name  
(type = character\*16, default = none)
- (2) EOS fluid sequence number<sup>2</sup>  
(type = integer, default = none)

#### Example

```
EOS_FLUID_ID 'Primary Fluid' 310
EOS_FLUID_ID Water 200
```

### EOS\_FLUID\_TYPE – EOS Fluid Database Information

Required

This record defines the fluid that will be loaded into the problem. The first two fields are required for all fluids.

- (1) EOS fluid database type
  - (a) BUILTIN
  - (b) TPF  
(type = character\*16, default = none)
- (2) EOS fluid database name  
Must be one of the database names are listed on Table 1.  
(type = character\*16, default = none)

The third field is only valid for TPF fluids and is optional:

- (3) TPF Filename  
(type = character\*80, default = listed on Table 1)

```
eos_input      ! Networks
! Fluids      eos_network_id    "ECCS-Network"  51
eos_fluid_id   "primary"      1      eos_network_cv    "eccs-1"
eos_fluid_type tpf      FLiBe      eos_network_fluid Water
!            !
eos_fluid_id   Water        18      eos_network_id    "Secondary-Network"  3
eos_fluid_type Builtin      Water    eos_network_cv    "eccs-2"
!            eos_network_fluid "eccs-2-fluid"
eos_fluid_id   "eccs-2-fluid" 26      eos_network_id    "Primary-Network"  498
eos_fluid_type tpf      Na      "na.tpf"      eos_network_cv    "primary"
!            eos_network_fluid "primary"
```

### EOS\_NETWORK\_ID – User Network Name and Sequence Number

Required

This record defines a unique, user-defined name for the network and a user-defined sequence number.

- (1) EOS network name  
(type = character\*16, default = none)
- (2) EOS network sequence number  
(type = integer, default = none)

#### Example

```
EOS_NETWORK_ID 'Primary' 310
EOS_NETWORK_ID Secondary 100
```

### EOS\_NETWORK\_CV – EOS Network Control Volume

Required

This record gives the control volume name that will act as the starting point for the EOS network search, which is described in subsection 1.1 of this UG. If the control volume name does not exist or the control volume belongs to another EOS network, the code will generate an input processing error.

- (1) Control Volume name  
(type = character\*16, default = none)

#### Example

```
EOS_NETWORK_CV 'Lower Head'
EOS_NETWORK_CV IRWST
```

### EOS\_NETWORK\_FLUID – EOS Network Fluid

Required

This record gives the EOS fluid name that will be used to select the EOS for the network. The EOS fluid name on this record must match one given on an EOS\_FLUID\_ID record or an input processing error will be issued.

- (1) EOS fluid name  
(type = character\*16, default = none)

#### Example

```
EOS_NETWORK_FLUID 'Primary-fluid'
```

# EOS – MELGEN Output



## Display information about EOS and networks

- EOS processes/checks on MELGEN pass 2
- EOS package gives results of network accounting
  - Whether EOS package input invoked or not
  - Check work if explicitly specifying EOS networks
  - Information on CV/FL and HS surface association
- Confirms condensable fluid for each EOS network
  - Echo/confirm if EOS input invoked
  - “legacy EOS” otherwise, CVH confirming fluid

```
Diagnostics during PASS2 input processing CVH package:
*****USING FLUID NAMED = Flibe !*****
NO Errors during PASS2 input processing CVH package
```

- Coming soon...EOS data on fluids in output

```
EOS Network Information
=====
Number of Subnetworks: 3

Network: Default Network 1
-----
ID: 1
Fluid: Legacy EOS
Control Volumes:
- Distrib_100 (100)
  - Root CV
  - Connected to Annulus_105
  - Connected to ColdLeg_330
```

```
Diagnostics during MELGEN Pass 2 input processing of EOS package
INFO: created default EOS network not specified in input.
      Network named 'Default Network 1' with root CV 'Distrib_100'
INFO: created default EOS network not specified in input.
      Network named 'Default Network 2' with root CV 'Sec_in'
INFO: created default EOS network not specified in input.
      Network named 'Default Network 3' with root CV 'Dummy'
No Errors during MELGEN Pass 2 input processing of EOS package
```

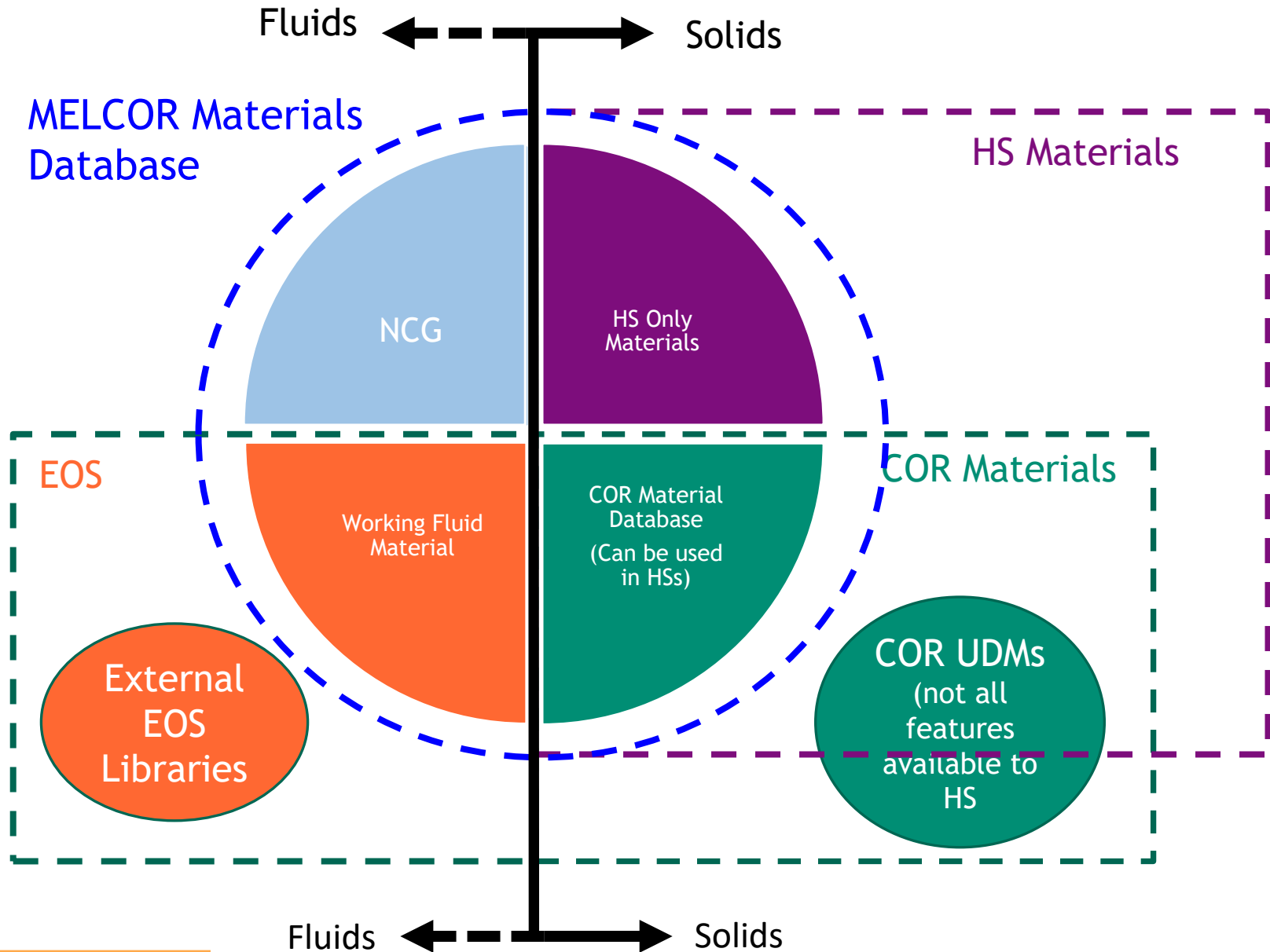
```
ID: 2
Fluid: Legacy EOS
Control Volumes:
- Sec_in (400)
  - Root CV
  - Connected to Sec_401
- Sec_401 (401)
  - Connected to Sec_in
  - Connected to Sec_402
- Sec_402 (402)
  - Connected to Sec_401
  - Connected to Sec_out
- Sec_out (403)
  - Connected to Sec_402
```

```
Flow Paths:
- Sec_400 (400)
  - Connected to Sec_in
  - Connected to Sec_401
- Sec_401 (401)
  - Connected to Sec_401
  - Connected to Sec_402
- Sec_402 (402)
  - Connected to Sec_402
  - Connected to Sec_out
```

```
Heat Structures Left Sides:
- HXtube3200 (3200)
  - Convects to Sec_401
- HXtube3211 (3211)
  - Convects to Sec_402
```

```
Heat Structures Right Sides:
(None)
```

# Diagram of MELCOR Materials - COR





# COR - Materials



## COR and non-hydrodynamic materials

- Either built-in/default, modified built-in/default, or new/user-defined
- In any case, materials are known to the MP package
- MP definitions of COR materials are held to comparatively strict requirements
- Exercise care with enthalpy function for COR materials (UDMs or redefined materials)
  - CPS and ENH are defined by *independent* tables, which must be consistent
  - Table for ENH must be consistent with MLT and LHF
  - Furthermore, LHF must be added between  $T = T_{MLT}$  and  $T = T_{MLT} + 0.01$  K in the ENH table
- Will review topics related to non-hydrodynamic COR materials
  - Primary materials as a concept
  - Material substitutions/redefinitions
  - User Defined Materials (UDM) – defaults, templating, and other capabilities
  - Eutectics model
  - Generalized oxidation model
  - Miscellaneous topics (secondary candling, hold-up, COR ejection, decay heat, emissivity, etc.)

COR interacts with condensable/noncondensable hydrodynamic materials (pool or atmosphere) in control volumes only indirectly through component surface interactions like heat transfer and oxidation

---

# COR – Primary Materials



Components have “primary materials” - Rigorous definition difficult to pose

- If a component has only one material, that one is the primary material of that component
- Usually, the primary material comprises most of the component mass and predominantly determines component properties (those that depend on material composition at least)
- Otherwise, think of primary material in a component and in a core cell as  
“the dominant material associated with a component surface in a COR cell before oxidation”
- Once oxidation begins, primary material may no longer be the main or only material associated with the component surface as primary materials are generally oxidizable
- Concept applicable to intact components...distinctions break down for PD/PB and MP

A heuristic definition: primary material is “where the action is” in a component

- Fuel primary material is where fission and energy generation occurs, holds/releases RNs
  - Clad primary material is what does heat transfer, oxidation, gap release, candling, collapse...
  - Core support primary material is what lends support
  - Nonsupport primary is the control poison that can melt and oxidize
  - Primary materials govern important behaviors (CS/NS collapse, oxide shell hold-up, ...)
  - Oxides (solid products of oxidation) aren’t primary materials but primary material oxides
-

# COR – Inputs for Material Substitutions



Materials can be replaced globally or specifically assigned to components

- COR\_MAT or simple MP input accomplishes the former,
- COR\_XXM accomplishes the latter

MP input – Universal “swap”...alter “thermal EOS” of  $mat_A$  for all purposes

COR\_MAT (COR\_RT) – COR “swap”...  $mat_A$  becomes  $mat_B$  for COR purposes

- $mat_A$  is still  $mat_A$  in MP (no redefinition of  $mat_A$  necessary)
- $mat_B$  has own definition in MP and simply replaces  $mat_A$  wherever it appears

COR\_XXM – targeted “swap”...narrowly tailored for purposes of component XX

- XX usually receiving  $mat_A$  (often as “primary material”) will instead receive  $mat_B$
  - Many XX allowed, some exceptions (e.g. COR\_FUM), respects oxidation/ejection
-

# COR – MP Inputs for Material Redefinition



```
MP_ID      'CARBON-STEEL'
!  size
MP_PRTF    3 !n      prop      itbprp      cfkey
           1      CPS 'CPS CARBON ST'
           2      THC 'THC CARBON ST'      TF
           3      RHO 'RHO CARBON ST'
```

MP Input replaces CPS, THC, and RHO database properties for CARBON-STEEL reported in RM

The following materials, listed with their mnemonic identifiers, are defined in the Material Properties package:

1. Zircaloy (ZR)
2. Zirconium Oxide (ZRO2)
3. Zirconium Oxide (ZRO2-INT)
4. Uranium Dioxide (UO2)
5. Uranium Dioxide (UO2-INT)
6. Stainless Steel (SS)
7. Stainless Steel Oxide (SSOX)
8. Boron Carbide (B4C)
9. Boron Carbide (B4C-INT)
10. Silver-Indium-Cadmium (AGINC)
11. Uranium Metal (UMETL)
12. Graphite (GRAPH)
13. Concrete (CON)
14. Aluminum (ALUM)
15. Aluminum Oxide (AL2O3)
16. Cadmium (CADM)
17. Stainless Steel 304 (SS304)
18. Carbon Steel (CS)
19. Iron-Chromium Aluminum (FCA)
20. Iron-Chromium Aluminum Oxide (FCAO)

# COR – COR\_MAT for Material Swap



The user swaps an existing “native” COR material with any suitable material in MP

Once the swap is declared, the original material is unavailable for use in COR

Recent code improvements permit all materials properties to participate in swap

```
MP_ID 'ZIRCONIUM-OXIDE'          ! default
MP_ID 'URANIUM-DIOXIDE'         ! default
MP_ID 'ZRO2-INT'      !({      ! redefined
MP_PRC  5600.000    2502.000    707.0E+3    ! density, melting temperature, latent heat of fusion
!})
MP_ID 'UO2-INT'      !({      ! redefined
MP_PRC  10960.00    2502.000    274.0E+3    ! density, melting temperature, latent heat of fusion
...
...
COR_MAT  2                      ! CORMAT MATNAM
  1 UO2  'UO2-INT'
  2 ZRO2 'ZRO2-INT'
```

**UO2 Material is no longer available for use in COR**

```
COR_KFU  2 !({ !Even though input card specifies UO2, UO2-INT is substituted
!      n IA IR XMFUO
  1 7 1 12000.
  2 7 2 12000.
```

# COR – COR\_XXM for Primary Materials



See COR UG for various COR\_XXM

- FU has special interpretation
- CL, MX, CN, SH, RF, HR, HP, FM, CS, NS
- Updated for allowed primary materials and oxides according to XX

Recent code improvements allow all material properties to participate in the primary material swap for XX

COR\_KXX and/or COR\_NMAT

- Populate XX with material mass
- If a UDM is the new primary, use COR\_NMAT for material mass in XX
- See COR\_UG

## Defining Primary Material

```
COR_KCL 12
!      IA IR XMCLZR XMCLZX XMCLIN
      1  1  1  0.0  0.0  1.972E-2
      2 2-15 1  0.0  0.0  1.183E-2
      3  16  1  0.0  0.0  1.183E-2
...
COR_CLM INC
```

## Defining Extra Fuel Material

```
COR_KFU 12
!      IA IR XMFUZO XMFUHT XMFUXM XMFUXO
      1  1  1  1.389E-2  0.0  1.215E-1
      2 2-15 1  8.332E-3  0.0  7.292E-2
      3  16  1  8.332E-3  0.0  7.292E-2
...
COR_FUM INC
```

# COR – User Defined Materials (UDMs)



COR utilizes what is declared purely through MP

UDMs have unique MATNAM and MPSHORT from MP\_ID

UDMs for COR use:

- Take one of four USERCORMATTYPE options
- Require some “material behavior” input:
  - If no MP\_BHVR input, default UDM behavior:
    - USRM1 and USRM2 are ‘STAINLESS-STEEL’
    - USRM3 and USRM4 are ‘ZIRCALOY’ and its oxide
    - Any MP changes to SS and ZR/ZROX carry through
  - If MP\_BHVR indicates, can “template” behavior:
    - All properties borrowed from another MP material
    - Can edit individual properties thereafter
    - Applicable to other non-COR USERCORMATTYPE
  - If MP\_BHVR “templates itself”:
    - MP\_PRTF and MP\_PRC required
    - May configure oxidation
    - May configure ejection group
- See MP\_BHVR in MP UG
- Viscosity
- Thermal expansivity
- COR emissivity

## USERCORMATTYPE

This word defines an identity for the type of user-defined material to be defined. Four options can be input so that the user-defined material specified on Field 1 can become associated with the COR Package, which may be allocated specific attributes as given by the options below. If options (a)-(d) are provided as input, then the material can be used in the COR and HS Packages.

(a) COR-USER1 or 1

Assign the material to the first generic COR material.

(b) COR-USER2 or 2

Assign the material to the second generic COR material.

(c) COR-USER-METAL or 3

Assign the material to a generic oxidizable COR material.

(d) COR-USER-OXIDE or 4

Assign the material to a generic oxide COR material.

```
! COR User-Defined Material
MP_ID      NewZirc  COR-USER-METAL  NUZR
MP_BHVR    Zircaloy  METAL  OXIDATION-MODEL  EXEMPT
MP_BETMU   1.65E-5   3313.0  1.076E-3
MP_COREMIS CF  'NewEmissivity'  0.0001  0.9999
! Initialize Mass in component
COR_NMAT 1 ! IA  IR  IC  USRM1  USRM2  USRM3  USRM4
          1  ALL  ALL  CL  0.0    0.0    64.2   0.0
! Associate with metal pool
COR_LAY 1 ! LAYMAT  MPLAY
          1  NUZR   UPPER  ! Associate with MP2
```

# COR – Eutectics Model Overview



## Eutectic reactions

- Low-melting-point mixtures at the interface between two or more materials
  - Boron carbide & stainless steel (control rods)
  - Uranium dioxide and zircaloy
  - Iron & molten uranium
- Can significantly affect core degradation processes
  - Fuel/Clad interactions ( $\text{UO}_2/\text{Zr}$ )
  - Early dissolution in B<sub>4</sub>C/SS control rods
  - Eutectic reaction between U and Fe leads to early clad dissolution in metal fuel systems

## SOARCA used interactive materials (e.g. $\text{UO}_2\text{-INT}/\text{UO}_2$ on COR\_MAT)

- Limited ability to capture eutectic effects
- $\text{UO}_2\text{-INT}$  and  $\text{ZRO}_2\text{-INT}$  used to reduce melt temperature and modify enthalpy curves
  - Alternate approach short of a better model/treatment
  - Applied globally to intact and conglomerate fields
- Effective melt temperature was user specified with no default
- **No Longer Best Practice**

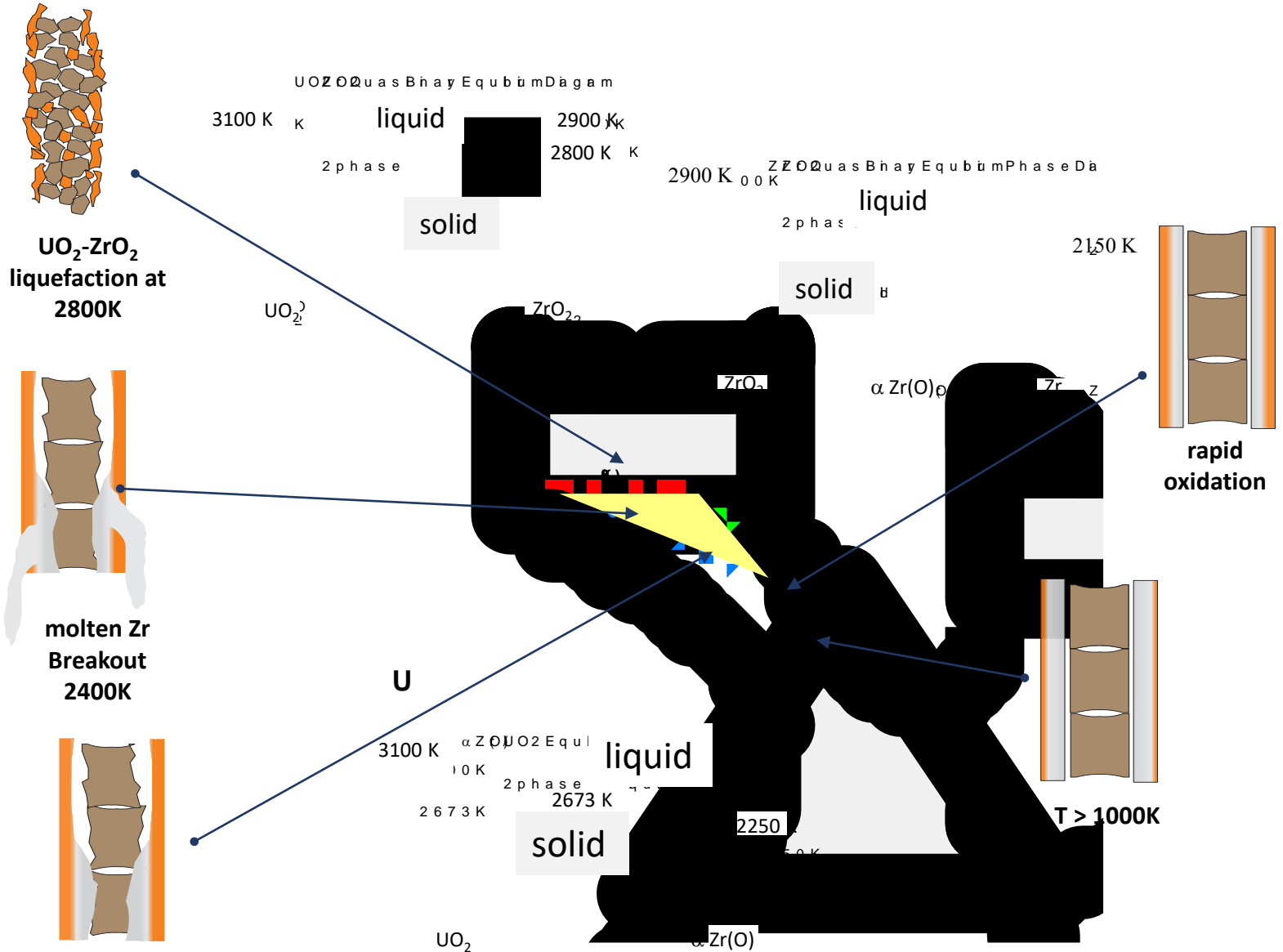
## Current Best Practice is to utilize the eutectics model

- Only applies to conglomerate
  - Liquefaction of solids in contact using calculated rates
  - Current code default
-



# COR – Eutectics Model

## U/Zr/O Ternary Phase Diagrams



# COR – Eutectics Model

## Effective Melt Temperature

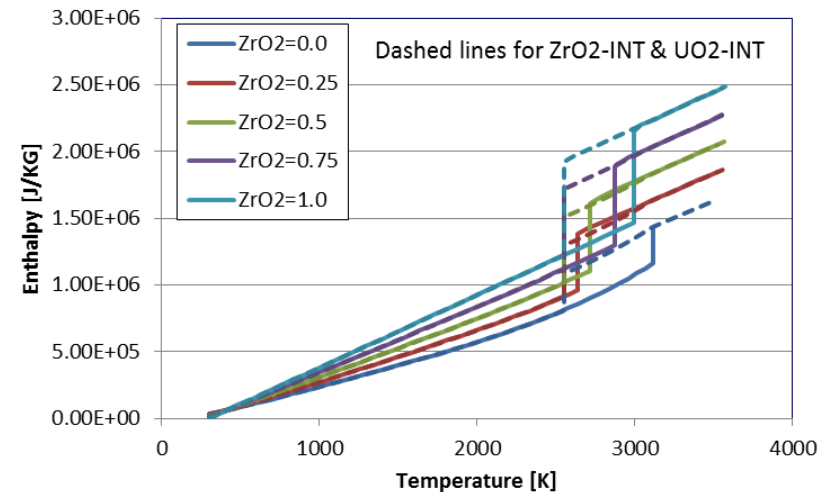
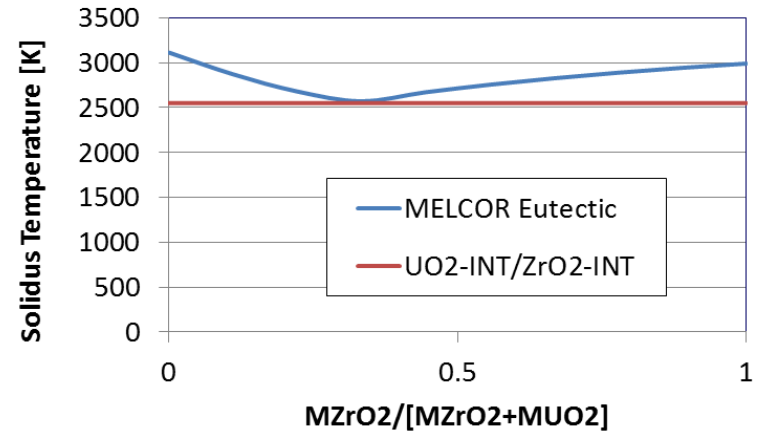


### Interactions model (UO<sub>2</sub>-INT/ZRO<sub>2</sub>-INT)

- Melt temperature for UO<sub>2</sub> and ZRO<sub>2</sub> is the same whether intact or conglomerate
- No composition dependency
- With this model, cannot enforce lower effective melting temperature
- UO<sub>2</sub>-INT and ZRO<sub>2</sub>-INT melt temperatures changed through user input

### Eutectics model

- Elemental melt points for intact material
- Eutectic temperature for conglomerate
- Compute liquefaction of solids in contact from calculated rates
- Melt temperature depends on composition



# COR – Eutectics Model

## Eutectic Mixtures



### Eutectic mixture composition

- Conglomerate debris materials associated with any intact component are treated as part of a coherent mixture
  - Some materials in mixture are mutually miscible
  - Other in mixture are mutually immiscible (i.e. they melt/relocate independently of each other)
- As currently implemented, when the model is active all materials part of miscible mix

### Formation of eutectic mixtures

- Normal liquid formed when an intact solid reaches its melting point
  - Eutectic reaction product formed when two intact solids in mechanical contact within a core component reach their eutectic temperature
  - Dissolution of an intact solid by an existing liquid mixture in the same core cell
    - Example: dissolution of  $\text{UO}_2$  (intact solid) by the liquid mixture associated with clad in same cell
    - At most, two distinct solids (hierarchy for dissolution)
-

# COR – Eutectics Model

## Dissolution of Solids by Molten Mixtures



Dissolution proceeds until

- Addition of solid lowers the updated gross mixture enthalpy to liquidus of the same, or
- Parabolic rate limitation associated with the dissolution reaction has been exceeded for the time-step

Solution is iterative

Component	Solids Dissolved by Mixture
Cladding	UO <sub>2</sub> from intact fuel
	ZrO <sub>2</sub> from intact cladding
Canister	ZrO <sub>2</sub> from intact canister
	ZrO <sub>2</sub> from intact cladding
	UO <sub>2</sub> from intact fuel
Other structure SS or NS (steel only)	steel oxide from the same other structure
Other structure NS (BWR control rod)	steel oxide from the same other structure
	ZrO <sub>2</sub> from intact canister
	Zr from intact canister
Other structure NS (PWR control rod)	steel oxide from the same other structure
	Zr from the same other structure
	ZrO <sub>2</sub> from intact cladding
	UO <sub>2</sub> from intact fuel
Particulate debris	UO <sub>2</sub> from particulate debris
	ZrO <sub>2</sub> from particulate debris
	ZrO <sub>2</sub> from intact cladding
	UO <sub>2</sub> from intact fuel

$$(x_j^f)^2 = (x_j^i)^2 + K_j \Delta t$$

$$K_j = A_j \exp(B_j / T)$$

where

$x_j^f$  = final mass fraction of material j,

$x_j^i$  = initial mass fraction of material j,

$\Delta t$  = timestep (s), and

$$A_{ZrO_2} = 1.47 \times 10^{14}$$

$$A_{UO_2} = 1.02 \times 10^{15}$$

$$B_{ZrO_2} = 8.01 \times 10^4$$

$$B_{UO_2} = 8.14 \times 10^4$$

# COR – Eutectics Model

## Eutectic Model Input



### New input for the eutectics model

```
COR_EUT 1 ! PairMelt    TM    F1
          1 'UO2/ZRO2' 2550.0 0.5
```

```
COR_EUT 0 ! Enables w/ defaults
```

- PairMelt one of following:
  - ZR/SS | 1 ; ZR/INC | 2 ; UO2/ZRO2 | 3
  - TM is solidus temperature for the eutectic pair
  - F1 is the molar ratio of the 1<sup>st</sup> member in the pair at the eutectic temperature

### Obsolete input for eutectics model

```
COR_MS IEUMOD
```

Message will indicate new input method.

ERROR: The Eutectics model is enabled on COR\_EUT

### Interactive materials model available, but not for use alongside eutectics model

```
MP_INPUT
  MP_ID 'ZRO2-INT'
    MP_PRC 5600.0 2502.0 707000.0 ! density, melt temp, latent heat
  MP_ID 'UO2-INT'
    MP_PRC 10960.0 2502.0 274000.0! density, melt temp, latent heat
COR_INPUT
  COR_MAT 2      !      CORMAT      MATNAM
            1      UO2      'UO2-INT'
            2      ZRO2      'ZRO2-INT'
```

These records should be removed from input

# COR – Eutectics Model



## Calculation of Mixture $T_{sol}$ and $T_{liq}$

Determine for given mixture by considering every binary combination of material pairs in the mixture (molar-weighted combination of solidus temperatures), i.e.:

$$T_{sol,mix} = \frac{\sum_j \sum_{i \neq j} (f_i f_j T_{sol,ij})}{\sum_j \sum_{i \neq j} (f_i f_j)}$$

- For eutectic pair  $(i, j)$  get  $T_{sol,ij}$  by the lever rule:
  - $T_{sol,ij}$  is mole-weighted average of the pair's eutectic temperature and the solidus temperature of the component present in excess of the eutectic molar composition

Material Pairs		Molar Ratio	Eutectic Temperature
Zr	Inconel	0.76 / 0.24	1210
Zr	steel	0.76 / 0.24	1210
ZrO <sub>2</sub>	UO <sub>2</sub>	0.50 / 0.50	2800
Zr	B <sub>4</sub> C	0.43 / 0.57	1900
Steel	B <sub>4</sub> C	0.69 / 0.31	1420
Zr	Ag-In-Cd	0.67 / 0.33	1470

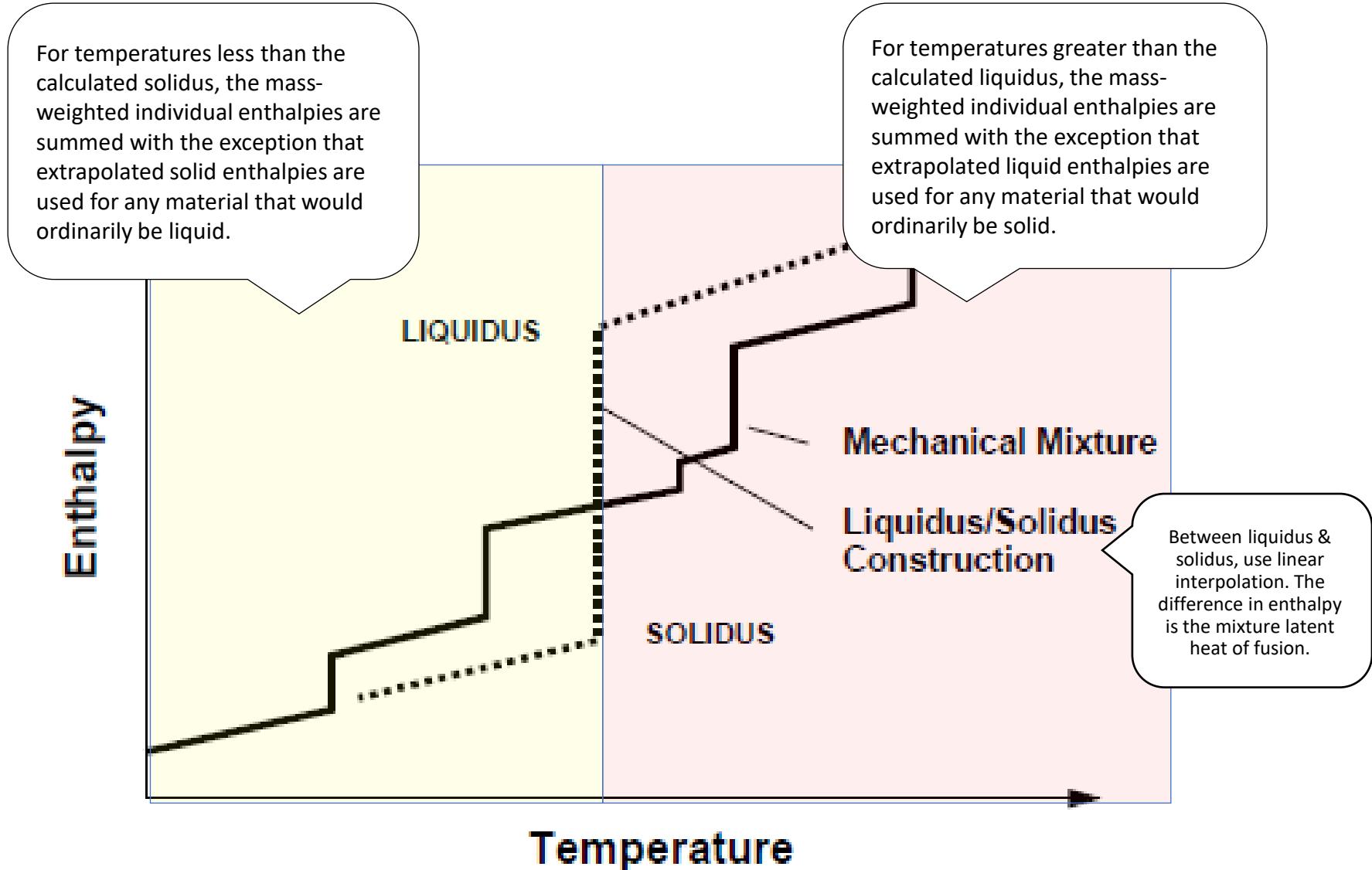
- For non-eutectic pair  $(i, j)$  get  $T_{sol,ij}$  by mole-weighted average of  $T_{sol,i}$  and  $T_{sol,j}$

$T_{liq,mix}$  set equal to  $T_{sol,mix}$  plus 0.01 K

---

# COR – Eutectics Model

## Calculation of Mixture Enthalpy



# COR – Eutectics Model

## TMI-2 Melt Progression



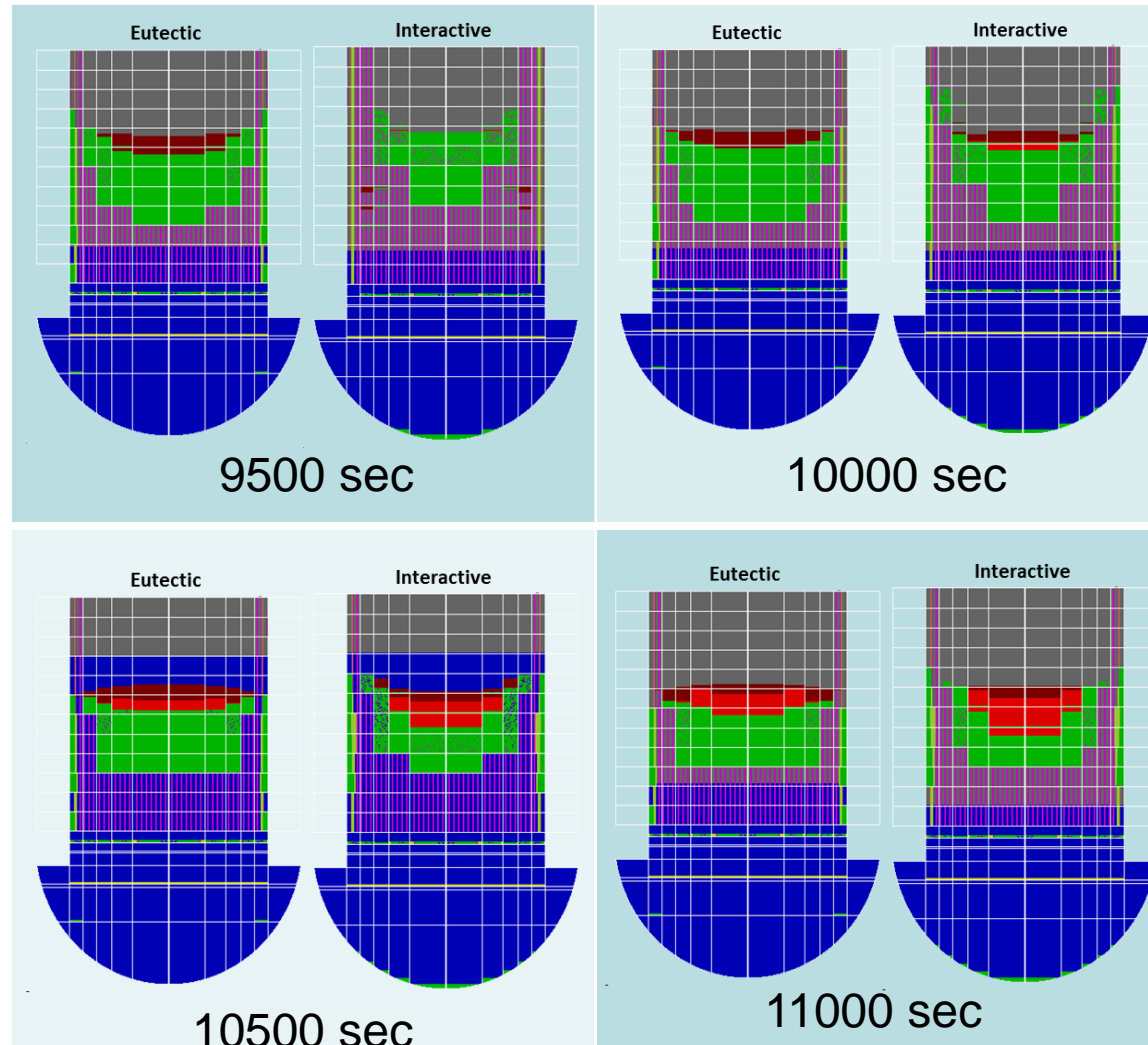
Compare 2 TMI-2 test cases

- Eutectics point – 2550 K
- $\text{UO}_2\text{-INT/ZRO}_2\text{-INT}$  – 2550 K

Some notable differences

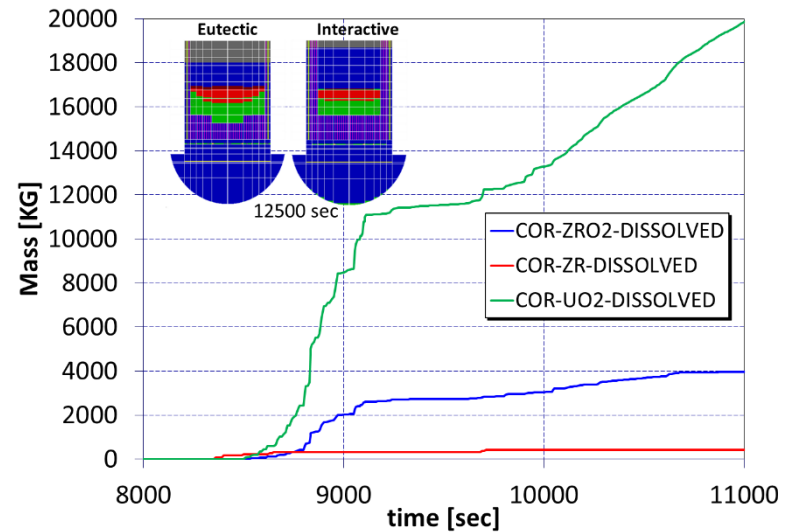
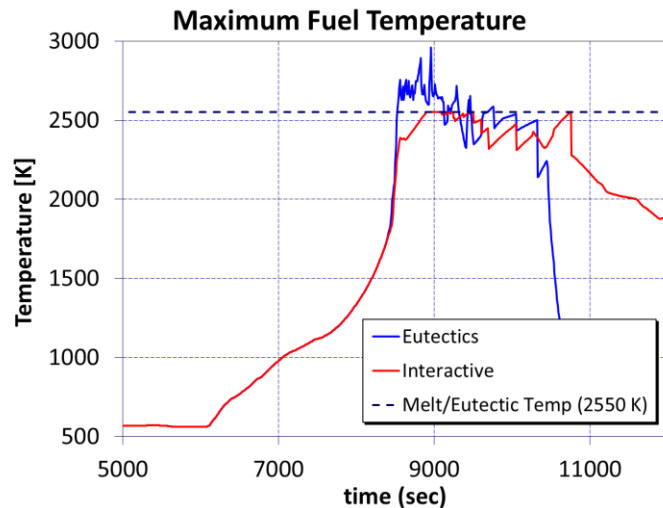
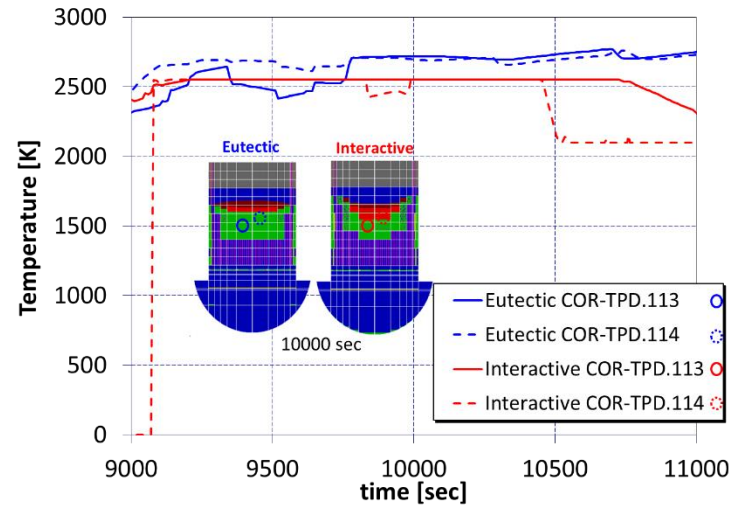
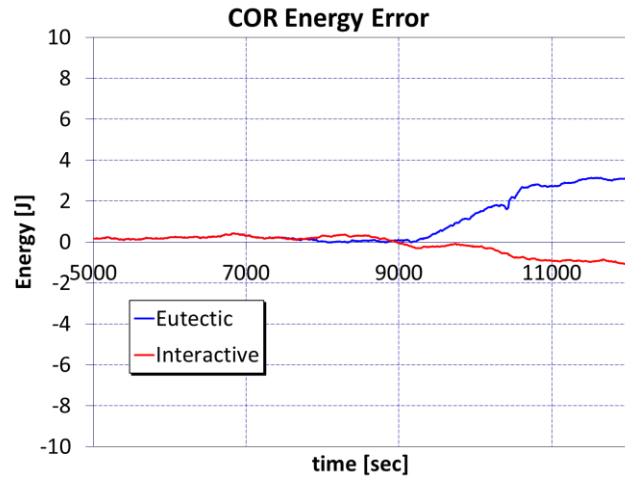
- Core damage > eutectics
- Molten pool size
  - Early on, > interactive
  - Later on, > eutectics
- Lower plenum relocation greater for interactive

Results are preliminary





# COR – Eutectics Model TMI-2 Melt Progression



# COR – Generalized Oxidation Model (GOM)



## Introduction

Historically, a specific set of materials (Zr, Stainless Steel, graphite, B4C, Al) could oxidize according to prescribed oxidation models

GOM utilizes UDMs to create new oxidizable materials with customizable oxidation rules (reactions, kinetics, ...)

- COR-USER-METAL or UDM3 is the oxidizable material
- COR-USER-OXIDE or UDM4 is its oxide
- Note UDM3 may not actually be metal
- Note UDM4 is not required to exist
- User has control over properties
- Oxidation behavior can be templated

GOM can overwrite default oxidation models for otherwise default materials

---

```
MP_ID FeCrAl COR-USER-METAL UFCA
MP_BHVR Itself METAL OXIDATION-MODEL
EXEMPT
MP_BETMU 3.1e-5 7.7 3313. 1.076e-3
MP_COREMIS linear - 0.0001 0.9999
0.042003702 0.0003474
MP_PRTF 4 ! NPAR PROPERTY DEFAULT/TF/CF (may
be only for THC)
1 ENH FCA-IntEn
2 CPS FCA-SpHeat
3 THC FCA-Conduct TF
4 RHO FCA-Density
```

```
MP_ID FeCrAl-Oxide COR-USER-OXIDE UFCAO
MP_BHVR ITSELF
MP_PRC 5180.0 1901.0 687463.0 193.4102395
MP_COREMIS linear - 0.0 1.0 0.7 0.0
MP_BETMU 3.1e-5 7.7 3313. 1.076e-3
MP_PRTF 4 ! NPAR PROPERTY DEFAULT/TF/CF (may
be only for THC)
1 ENH FCAO-IntEn
2 CPS FCAO-SpHeat
3 THC FCAO-Conduct TF
4 RHO FCAO-Density
```

# COR – Generalized Oxidation Model (GOM)

## MELGEN Input



Assuming a UDM3 in MP with 'OXIDATION-MODEL' (and maybe UDM4 too), code expects COR input pursuant to oxidation model definition

COR\_GOX initiates an input block for a given material's oxidation rule(s)

- MATOX – identifies material UDM3/USRM3 in MP database
- GASOX – choose oxidant (oxygen/air or steam)
- OXIDE – identifies material UDM4/USRM4 in MP database (if present)
- TMIN – lower bound on MATOX/GASOX reaction(s) [K]
- TMAX – upper bound on MATOX/GASOX reaction(s) [K]

COR\_GOXMOL[n] defines stoichiometry of oxidation reaction sequence (1...n)

- NOXIDANT – oxidant moles consumed per one mole of MATOX consumed
  - NOXIDE – oxide moles produced per one mole of MATOX consumed
  - NCO, NCO2, NCH4 – product NCGs per one mole of MATOX consumed
  - ReacScale and ProdScale – see COR UG/RM for context and discussion
-

# COR – Generalized Oxidation Model (GOM)

## MELGEN Input



COR\_GOXPARG[n] defines parameters of the oxidation reaction sequence (1...n)

- If employing the reactant/product scalars:
  - QOX – Heat of reaction [J]
  - MnR – Gas diffusion constant setting oxidation diffusion limit [kg/mol/J]
- If instead specifying reactant mass fractions:
  - XR – Weight fraction of reactant n for MATOX
  - MWMET – Molecular weight of reactant n for MATOX [kg/mol]
  - MWOX – Molecular weight of oxide produced due to reactant n for MATOX [kg/mol]

COR\_GOXDB[n] defines reaction kinetics of the oxidation reaction sequence (1...n)

$$\frac{dW^n}{dt} = Ae^{-B/T}, \quad T_{min} \leq T \leq T_{max}$$

- Each reaction can have a piecewise temperature domain (NUMDOM)
  - TMIN\_DOM – Domain lower temperature bound
  - TMAX\_DOM – Domain upper temperature bound
  - A, B, n – Arrhenius parameters and kinetics parameter (e.g. n=2 for parabolic)
-

# COR – Miscellaneous Models

## Secondary Candling



### Eutectics model ON...

- Secondary candling inactive
- Eutectics model predicts material interactions

### Eutectics model OFF...

- Simple model for transport of unmelted material along with candling rivulets
  - $ZrO_2$ ,  $UO_2$ , steel oxide, control poison transported with candling molten material
  - Could model dissolution of  $UO_2$  by molten Zr or broken of  $ZrO_x$  shell
- Input fractions of secondary material transported
  - Fraction F1 of molten mass

$$\Delta M_s = F_1 \Delta M_m$$

- Fraction F2 of existing mass fraction within component

$$\Delta M_s = F_2 (M_{s,total} / M_{m,total}) \Delta M_m$$

---

# COR – Miscellaneous Models

## Oxide Shell Hold-Up



Molten material that would candle is “held up”

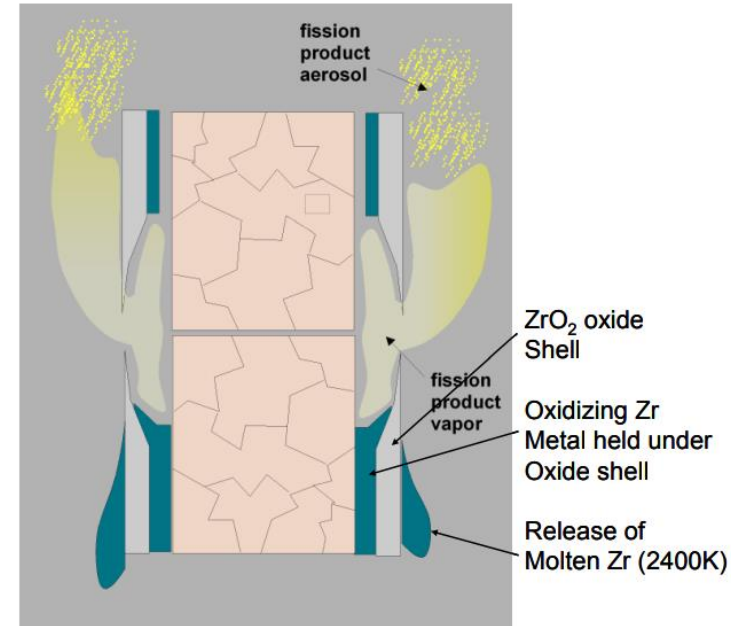
- Behind an oxide shell of thickness  $> \Delta r_{hold}$
- If component temperature  $< T_{breach}$
- If no candling from component has happened

Eutectics model...disregard dissolution by oxide

UDM considerations...

- Molten UDMs can be held up by oxide shell
- UDM4 (oxide) can hold up other-than-UDM3
- UDM4 hold-up subject to similar conditions

SC1131 for critical thicknesses & temperatures



Component	Solids Dissolved Effected by Oxide Layer
Canister	ZrO <sub>2</sub> from intact cladding (A)
Other structure NS (BWR control rod)	ZrO <sub>2</sub> from intact canister (A)
	Zr from intact canister (A)
Other structure NS (PWR control rod)	Steel oxide from the same other structure (B)
	ZrO <sub>2</sub> from intact cladding (A)
	UO <sub>2</sub> from intact fuel (A)

- solid is attacked only if there is no holdup of the mixture in the component.
- solid is attacked only if the mixture is being held up by the component

# COR – Miscellaneous Models

## COR Ejection



Conventional COR materials eject properly upon lower head failure and map into FDI or CAV (and Vanesa) via TP

UDMs not presently mapped into FDI/CAV

COR Material Index	Material	Ejection Group
8	ZIRCALOY	EJ-ZIRCALOY
9	ZIRCONIUM-DIOXIDE	EJ-ZIRCALOY
10	URANIUM-DIOXIDE	EJ-ZIRCALOY
11	STAINLESS-STEEL	EJ-STAINLESS-STEEL
12	STAINLESS-STEEL-OXIDE	EJ-STAINLESS-STEEL
13	BORON-CARBIDE	EJ-STAINLESS-STEEL
14	SIC	EJ-STAINLESS-STEEL
15	EUTECTIC	EJ-EUTECTIC
16	URANIUM-METAL	EXEMPT
17	GRAPHITE	EXEMPT
29	URANIUM-HEXAFLUORIDE	EXEMPT
30	ALUMINUM	EXEMPT
31	ALUMINUM-OXIDE	EXEMPT
32	CADMIUM	EXEMPT
33	STAINLESS-STEEL-304	EJ-STAINLESS-STEEL
34	LITHIUM-ALUMINUM	EXEMPT
35	URANIUM-ALUMINUM	EXEMPT
36	CARBON-STEEL	EJ-STAINLESS-STEEL
37	B4C-INT	EJ-STAINLESS-STEEL
38	ZRO2-INT	EJ-ZIRCALOY
39	UO2-INT	EXEMPT
All other indices	All other materials	EXEMPT

Materials in blue are “Ejection Group Leads”.

# COR – Miscellaneous Models

## Decay Heat, Fission Power, and Emissivity



Fission power and decay power absorption efficiencies:

- COR materials generally allowed to absorb some part of fission and decay power
  - SC1311 for fission power absorption by “native” materials and UDMs in indices 11-14
  - SC1322 for decay power absorption by “native” materials and UDMs in indices 11-14
- Absorption (fission or decay) only used if host components participate
- UDM templating extends to these absorption efficiencies

### 1311 – Material Fission Power Absorption Efficiencies

- (9) Core User1 efficiency  
(default = 0.0 BWR, or 0.0 PWR, units = none, equiv = FEFF(11))
  - (10) Core User2 efficiency  
(default = 0.0 BWR, or 0.0 PWR, units = none, equiv = FEFF(12))
  - (11) Core User Metal efficiency.  
(default = 0.0 BWR, or 0.0 PWR, units = none, equiv = FEFF(13))
  - (12) Core User Oxide efficiency.  
(default = 0.0 BWR, or 0.0 PWR, units = none, equiv = FEFF(14))
-



# COR – Miscellaneous Models

## Decay Heat, Fission Power, and Emissivity



COR material emissivity - SC1101-1109 for “native” and UDM material emissivity

COR-USER1 & COR-USER2

$$\varepsilon_{USER1} = C1106(2) + C1106(3)[T - 1106(1)]$$

$$\varepsilon_{USER2} = C1107(2) + C1107(3)[T - 1107(1)]$$

Calculated emissivity bounded by indices 4 and 5

- (1) Reference Temperature.  
(default = 616.4833, units = K)
- (2) Reference Value.  
(default = 0.25617, units = none)
- (3) Temperature coefficient  
(default = 0.0003474, units = K<sup>-1</sup>)
- (4) Maximum value.  
(default = 0.9999, units = K)
- (5) Minimum value.  
(default = 0.0, units = K)

COR-USER-METAL & COR-USER-OXIDE

Oxidation dependent on oxide thickness

Emissivity interpolation table (oxide thickness vs emissivity)

$\Delta\Gamma_{ox}$	$\varepsilon$
0.0	C1108(1)
C1108(2)	C1108(3)
C1108(4)	C1108(5)

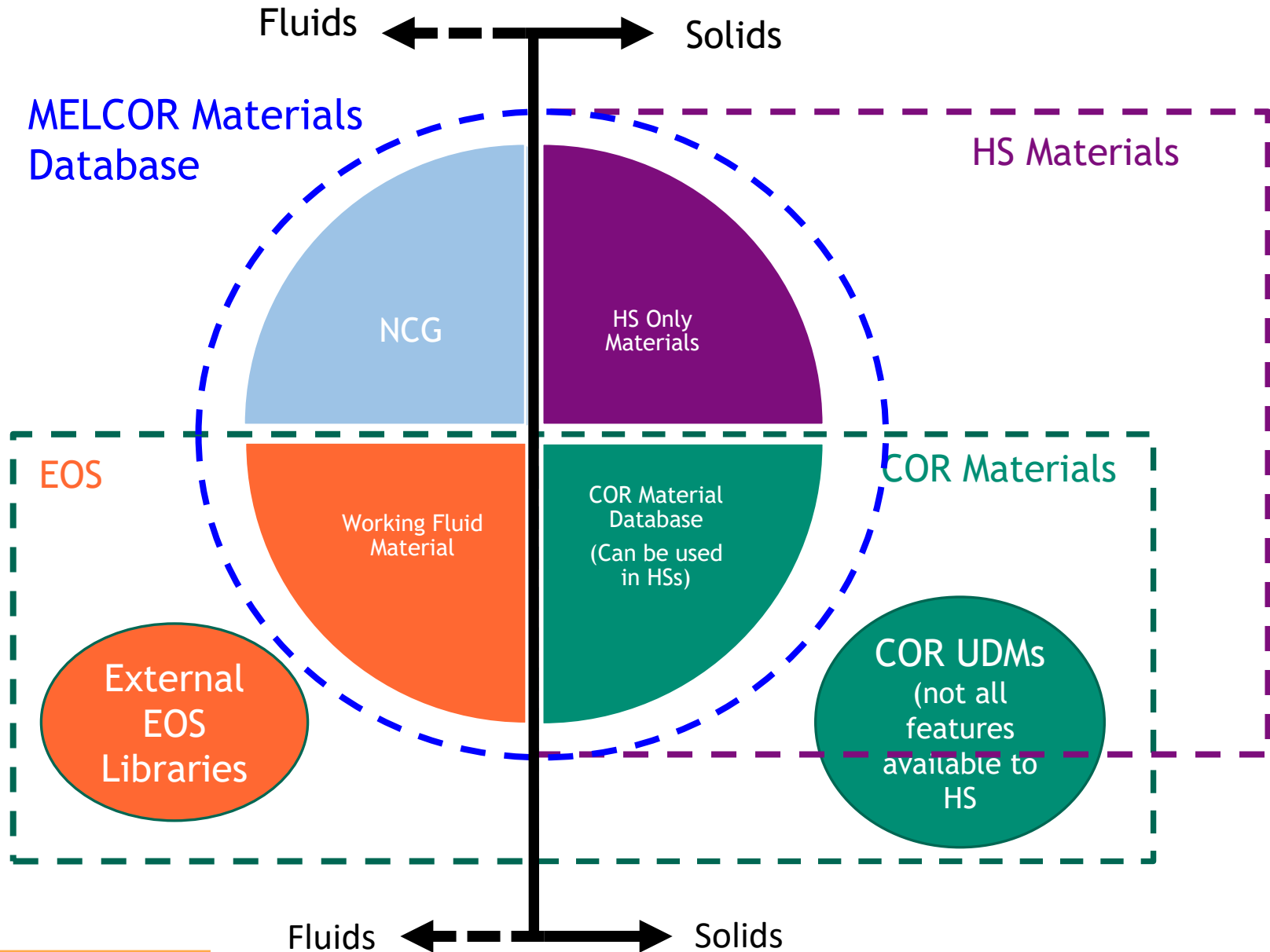
Oxidation dependence on temperature

$$\varepsilon(T > T_{max}) = \varepsilon \cdot \exp\left(\frac{C1108(6) - T_{max}}{C1108(7)}\right)$$

Calculated emissivity bounded by indices 8 and 9

- (1) Clean-surface emissivity.  
(default = 0.325, units = none)
- (2) Oxide thickness 1.  
(default = 3.8799999E-6, units = m)
- (3) Emissivity at oxide thickness 1.  
(default = 0.808448, units = none)
- (4) Oxide thickness 2.  
(default = 0.001, units = m)
- (5) Emissivity at oxide thickness 2.  
(default = 0.758642, units = none)
- (6) Temperature above which emissivity is degraded.  
(default = 1500.0, units = K)
- (7) Temperature range over which emissivity is degraded.  
(default = 300.0, units = K)
- (8) Maximum value.  
(default = 0.9999, units = none)

# Diagram of MELCOR Materials - HS



# HS - Materials



## HS and non-hydrodynamic materials

- Either built-in/default, modified built-in/default, or new/user-defined
- In any case, materials are known to the MP package
- MP definitions of HS materials not so stringent on enthalpy requirements
- Fabricate HS mesh intervals of MP materials
- Possible that non-hydrodynamic materials in HS become COR materials

## HS interacts with condensable and noncondensable hydrodynamic materials (pool or atmosphere) in control volumes

- Through heat and mass transfer processes at HS surfaces
  - Including film “surface nodes”
  - HS-2D may expand and complicate the interaction(s) somewhat
-

# Summary



MELCOR has an extensive database of built-in/default materials for:

- Non-hydrodynamic materials
  - COR materials
  - HS materials external to core
- Hydrodynamic materials
  - Condensable (one or more in a calculation)
  - Noncondensable (gases)

MELCOR can accept user input to modify existing materials or declare new ones

Many physics models intersect with materials modeling

---



- MELCOR has an extensive database of built-in materials used for characterizing
  - Core materials
  - Structural materials external to the core
  - Hydrodynamic materials.
- Furthermore, MELCOR user input can modify existing materials or fully specify new materials.
- Recent developments
  - COR Eutectics model
  - User-Defined Materials
  - Generalized Oxidation Model
  - User-defined EOS
  - Multiple condensable working fluids in a model (upcoming code release)